D-Alanine, N-(2,5-ditrifluoromethylbenzoyl)-, nonyl ester

Inchi: InChI=1S/C21H27F6NO3/c1-3-4-5-6-7-8-9-12-31-19(30)14(2)28-18(29)16-13-15(20(22,2

InchiKey: BNFUMRVSGIUGBI-UHFFFAOYSA-N

Formula: C21H27F6NO3

SMILES: CCCCCCCCCOC(=O)C(C)NC(=O)c1cc(C(F)(F)F)ccc1C(F)(F)F

Mol. weight [g/mol]: 455.43

Physical Properties

Property code	Value	Unit	Source
gf	-1219.98	kJ/mol	Joback Method
hf	-1766.53	kJ/mol	Joback Method
hfus	53.02	kJ/mol	Joback Method
hvap	80.40	kJ/mol	Joback Method
log10ws	-7.60		Crippen Method
logp	6.136		Crippen Method
mcvol	312.600	ml/mol	McGowan Method
pc	1085.63	kPa	Joback Method
rinpol	2218.00		NIST Webbook
rinpol	2218.00		NIST Webbook
tb	885.57	K	Joback Method
tc	1084.57	K	Joback Method
tf	546.02	K	Joback Method
vc	1.248	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1011.93	J/mol×K	885.57	Joback Method
cpg	1026.31	J/mol×K	918.74	Joback Method
cpg	1039.68	J/mol×K	951.90	Joback Method
cpg	1052.14	J/mol×K	985.07	Joback Method
cpg	1063.73	J/mol×K	1018.23	Joback Method
cpg	1074.54	J/mol×K	1051.40	Joback Method
cpg	1084.64	J/mol×K	1084.57	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U347804&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

Legend

cpg:	Ideal gas heat capacity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume